

INFLUENCE OF INPUT PARAMETERS ON THE FIRE SIMULATION

Trettin, C., Hagemann, P., Werrel, M., Meinert, M., Wittbecker, F.-W.

University of Wuppertal
Gaußstraße 20
Wuppertal, 42119, Germany
e-mail: trettin@uni-wuppertal.de

ABSTRACT

The use of computational fluid dynamics in fire safety engineering requires the applicability of the employed model according to a specific fire scenario. To be able to estimate how the simulation outcome is influenced by model assumptions and simplifications, the user has to evaluate the dominating physical processes and involved empirical parameter that has an essential influence on the specific fire scenario.

Thermogravimetric analysis (TGA) will be used to show in which ranges the input parameters ($T_{\text{reference}}$, Reaction Rate, Pyrolysis Range, Heating Rate...etc.) in a fire simulation with the "Fire Dynamics Simulator" will vary based on the measurement errors, measurement uncertainty, or misinterpretation of the user. The impact of those variant input parameters on the simulation of one specific fire scenario will be evaluated and will be discussed. Additionally, the influence of model assumptions (e.g. SOLID_PHASE_ONLY=.TRUE.) to validate the TGA together with fixed material properties on the simulation result will be carved out.

To calculate the fire spread in a simulation, chemical and thermal material properties are analyzed by the use of the Cone Calorimeter and TGA in their different laboratory scales.

Additionally to the measurement conditions and model assumptions, the user has to evaluate the material properties for simulation input according to their specific laboratory scale compared to the specific fire scenario that should be simulated. For this purpose, different virtual scales are used to discuss the influence on the simulation of the fire dynamics simulator.

INTRODUCTION

To model fire spreading in real scale scenarios the user determines especially the material input parameter from literature respectively from laboratory scales. Usually, the input parameters will be validated by modeling the laboratory scale experiments, like the cone calorimeter or thermogravimetric analysis. Afterwards the input parameter will be transferred into the real scale scenario or user specific fire scenario. Different references^{1,4,7} show the challenge of modeling and

reproducing a real experiment with FDS. The approach to implement data from laboratory scale experiments requires the knowledge about the fire behavior of the used materials and also about the transferability of the experiments to the considered fire scenario. In this work the results of thermogravimetric analysis and cone calorimeter experiments will be discussed. The second part will focus on the comparison of the modeled results by FDS 6.1 with experiments. Concluding, the influence of the input parameter and the consequences of the simulated results will be discussed.

EXPERIMENTS

To simulate fire spreading with the pyrolysis model of FDS, thermogravimetric analysis for selective materials were conducted: flexible foam (polyurethane, PU), LEGO® brick (acrylonitrile-butadiene-styrene copolymer, ABS), black polymethyl methacrylate (PMMA) and particle board are examined. With a heating rate of 5 K/min and 60 K/min for selected samples, the different derived pyrolysis parameters will be compared. The temperature of the test series range from 50 °C to 1000 °C, conducted with crucibles of 70 µl and 150 µl. During the thermogravimetric analysis of ABS and PU the ambient conditions vary between 10 % and 21 % oxygen concentration.

The different test samples are sub-divided into charring (Particle board, PU) and melting (PMMA, ABS) samples³. This classification helps to characterize the typical fire behavior, to validate the experimental results (TGA) and to model the FDS simulation.

Charring materials produce a barrier between the pyrolysis zone and the exposed surface. The process of decomposition will be reduced depending on the properties of the material, the char and heat source.³ The user of FDS should implement the residue of the charring and needs to be aware, that breaking the char layer during the decomposition cannot be modeled.⁶ Considering additionally layers for modeling the producing and breaking of char layers helps to take the effects of the combustion into account.

Melting is an endothermic process, which leads to a liquid material. Modeling this effect is currently

impossible with FDS⁶: The user needs to characterize liquid properties (e.g. boiling temperature) for the sample, although the initial state is solid.

Flexible Foam / Polyurethane (PU)

The flexible foam is commercially available and consists mainly of PU. Because of that a decomposition of polyol-isocyanate, will be expected, which leads to liquid polyol (continues decomposing) and vaporized isocyanate¹⁰. This is visualized by two reactions shown in figure 1. Here the normalized mass fraction (left hand y-axis blue line) and the reaction rate (right hand y-axis red line) of PU is plotted against the temperature.

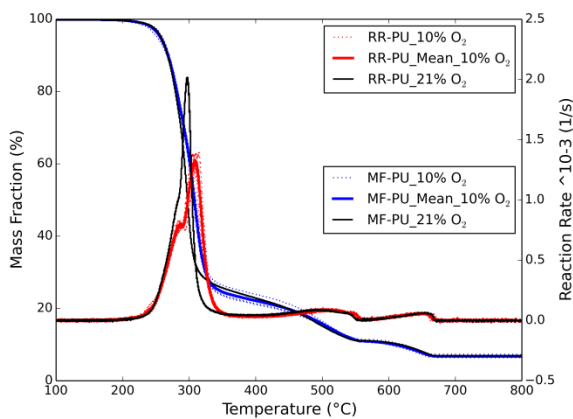


Figure 1: Normalized mass fraction and reaction rate of PU for different oxygen concentrations by 5 K/min

It can be observed that with respect to the temperature in total four reactions take place: The first reaction ranges from 210 °C to 295 °C with a mass lost of 28 % to 30 %. The second peak reaches from 290 °C to 380 °C. These results are similar to literature references^{8,9,11} and advise to a composite of toluene diisocyanate (TDI) and polyether¹¹. Totally 7 % of the original mass is residue. Because of the unknown additions through the suppliers the third (450 °C - 560 °C) and fourth (610 °C - 680 °C) reactions are not typical for flexible foam. The standard deviation of the mass loss lies by 3.21, while the reaction rate is lower than 0.15, which shows a good reproducibility of the thermogravimetric analysis. For an oxygen concentration of 21 % the temperature range of the pyrolysis decreases in comparison to an oxygen concentration of 10 %. On the other hand, the reaction rate increases. In conclusion, the sample reacts more rapidly with increasing oxygen concentration.

LEGO® Brick/ Acrylonitrile-butadiene-styrene copolymer (ABS)

ABS, which is classified as thermoplastic³, melts before vaporization without leaving significant residue (< 0.5 %). The LEGO® brick shows four to six reactions, although only two are dominant, shown in fig. 2. Compared to literature references, the pyrolysis process starts 200 °C earlier than it was measured and tabularized before³. The standard deviation is lower than 3.21 for the mass loss and 0.28 for the reaction rate. Here, the comparison between the different oxygen concentrations of the environment shows no significant differences. This could be explained by the very good ratio of sample surface to oxygen, as the inside of the sample is a hole and filled with ambient oxygen condition.

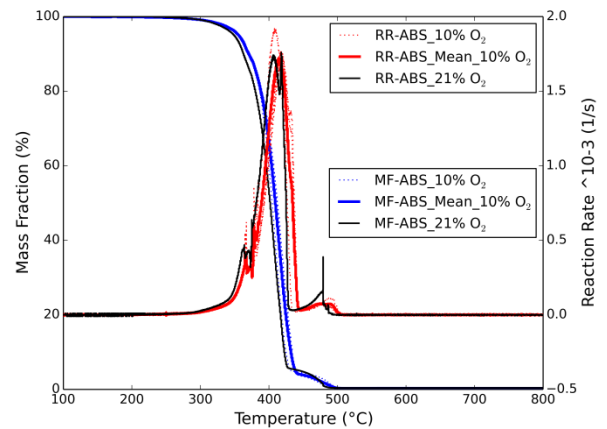


Figure 2: Normalized mass fraction and reaction rate of ABS for different oxygen concentrations by 5 K/min

Particle Board

Due to the different materials like wood and adhesives the specific composition of particle boards is unknown. In conclusion the pyrolysis will proceed individually. However, the reference⁵ shows the same trend of the reaction rate and distinguishes between (1) the desorption of bounded water, (2) the development of volatile products and (3) the formation of char. These simplifications of the pyrolysis processes are reflected by the TGA for the temperature range (1) ~ 100 °C, (2) 200 °C – 350 °C and (3) 360 °C – 490 °C. As shown in figure 3, the influence of the heating rate is significant. With an increasing heating rate, the decomposition starts at higher temperatures. Furthermore the charring process seems to disappear, though the mass fraction still reduces and the pyrolysis process is active. This behavior is also confirmed by reference³. Additionally, the temperature range of a reaction step enlarges and the reaction rate increases by ten times, while in contrast the percentage mass loss rate (not shown) decreases.

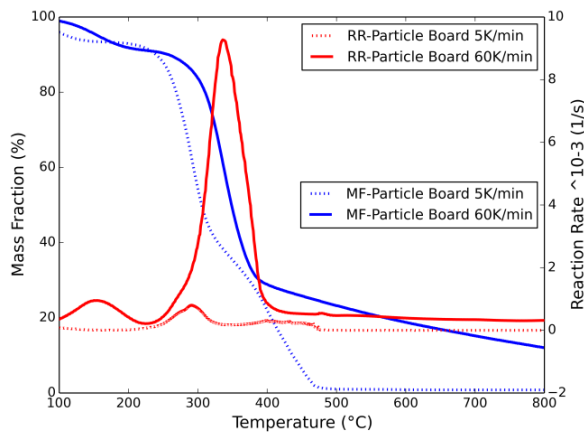


Figure 3: Normalized mass fraction and reaction rate of particle board for different heating rates by 21 % O₂ concentration

Polymethyl Methacrylate (PMMA)

Two blacked PMMA samples from different suppliers (A+B) were examined. Although the material is the same for each sample, the maximum reaction rate is nearly 0.002 (1/s) for sample A compared to 0.0015 for sample B. However, the decomposing starts and ends similar for both samples. The increasing heating rate during the thermogravimetric analyses of PMMA leads to the same behavior than the particle board. The graphs of the two samples of PMMA converge to each other.

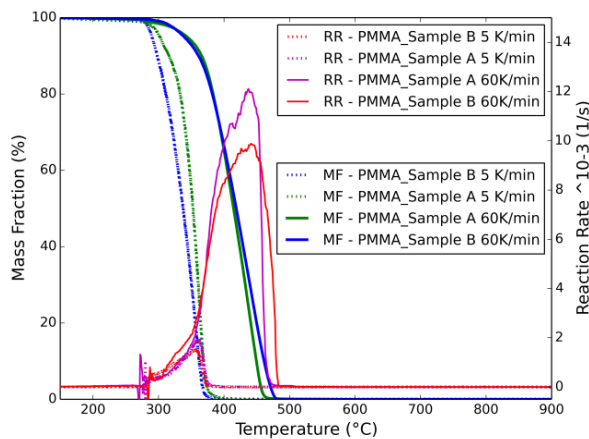


Figure 4: Normalized mass fraction and reaction rate of PMMA for different heating rates by 21 % O₂ concentration

In literature², PMMA is described as a simple decomposition with four to five steps of thermal degradation to monomers between 270 °C to 485 °C³. Due to the plateau of the reaction rate at the beginning of the pyrolysis of sample A, it is assumed,

that other additives during the manufacturing are contained. Primarily the first three steps of degradation between the samples distinguish from each other. As it can be seen in figure 4, the pyrolysis range extends from 270 °C to 390 °C for low heating rates and from 270 °C to 490 °C for the heating rate of 60 K/min. Additionally the reaction is more inactive at the lower temperatures during the higher heating rate, demonstrated by the normalized mass fraction in figure 4. The endothermic melting process leads to a nearly complete consumption of the fuel. Here, the residue lies below 0.1 %.

Results

The TGA reflects the typical reaction of the materials especially for a low heating rate. With an increasing heating rate, the fine resolution of the individual reaction steps gets lost (e.g. charring). This is due to the delayed heat up behavior of the sample (thermal inertia) compared to the heating rate of the oven and the reduced time for degradation steps. Furthermore, the temperature range of the decomposition and the reaction rates increases.

The change of the oxygen concentration influences the pyrolysis process, if the permeability of the material enables an increasing local oxygen concentration in the pyrolysis zone, in case the degradation depends on the oxygen concentration¹². For PU the influence of the oxygen concentration is higher than for ABS due to their material properties. The PMMA samples demonstrate possible different decomposition behavior for one material despite the same chemical classification. Because the chemical composition of the materials depends on the production/manufacturing methods or the various additives through the suppliers, the materials react differently. Consequently the transfer of tabularized material properties from literature to a specific simulation should be carried out carefully.

SIMULATION

The influences of the implemented model assumption and the input parameters are presented by adjusting the different models of FDS step by step.

Laboratory Scale

To simulate a real scale scenario the FDS Users Guide⁶ advises to test the pyrolysis model by a simple TGA example. Without modeling the gas phase, the focus lies on reproducing the mass loss rate respectively the reaction rate of the thermal gravimetric analysis. Because a very thin sample (1 mm) is modeled, the influence of the density, specific heat, conductivity of the sample is marginal and can be neglected. Furthermore, the influence of the grid on the results could be prevented by avoiding the

modeling of the gas phase. These assumptions allow to focus on the necessary pyrolysis parameters like the pre-exponential factor and reactions rate or alternatively, reference temperature and pyrolysis range.

Oxygen concentration

The TGA results of foam and LEGO® brick were modeled with FDS to obtain the Arrhenius parameters for the different conditions of the oxygen concentration. At first the input parameters, the rate of reaction and the corresponding temperature were delivered from the mass fraction of TGA. Afterwards the Arrhenius parameters are calculated by the implemented pyrolysis model of FDS. In the following table 1 these results are listed for PU and ABS.

Table 1: Arrhenius parameters of PU and ABS fitted by FDS

5 K/min	E (kJ/kmol)		A (1/s)	
	10 % O ₂	21 % O ₂	10 % O ₂	21 % O ₂
PU	1.98E+05	2.25E+05	6.92E+15	3.22E+18
	1.38E+05	1.05E+05	1.10E+10	2.94E+04
	1.35E+05	3.20E+05	3.12E+06	7.34E+15
	4.19E+05		4.55E+21	
ABS	2.49E+05	2.45E+05	1.07E+18	7.42E+17
	3.12E+05	1.90E+05	1.54E+23	9.11E+12
	2.56E+05	2.59E+05	9.56E+16	5.47E+17
	3.15E+05	5.40E+05	5.95E+19	7.09E+38
		5.10E+05		2.68E+33

It is obvious, that the degradation steps depend on the ambient conditions, which lead to different number of modeled reactions. However, it is important to reflect the characterized reactions of the considered material, e.g. two reactions of PU to polyol and isocyanate.

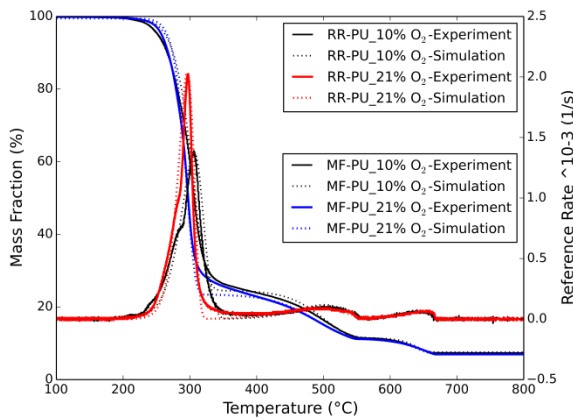


Figure 5: Comparison of PU simulation and TGA

Figure 5 shows exemplarily the plot of the simulated mass fraction and reaction rate compared to the TGA. Despite the very good agreement of the simulated TGA, the temperature range of the first reaction of

PU for oxygen concentration of 21 % is very small and cannot be reproduced by the simulation.

Heating rate

The same procedure as for the oxygen concentration was conducted for the different heating rates of the TGA. Table 2 shows the difference of the Arrhenius parameter between the heating rate of PMMA and particle board.

Table 2: Arrhenius parameters of PMMA and Particle Board fitted by FDS

21 % O ₂	E (kJ/kmol)		A (1/s)	
	5 K/min	60 K/min	5 K/min	60 K/min
Particle Board	2.6E+03	3.76E+04	7.95 E-04	1.09E+03
	7.18E+04	1.01E+05	1.02 E+04	1.39E+07
	5.05E+04	3.42E+04	1.00 E+01	3.38E-01
	3.82E+04		7.39 E-01	
	4.02E+04		5.80 E-01	
	4.12E+04		6.18 E-01	
PMMA B	1.54E+05	9.98E+04	2.78E+11	7.15E+05
	3.30E+05		2.93E+26	
	2.48E+05		2.66E+18	

With an increasing heating rate, the number of reactions is reduced. However, not every degradation step can be reproduced by the simulation. Because of that, the simulation simplifies the reaction of some materials, e.g. temperature range between 360°C and 490 °C of particle board could not be reproduced completely, as shown in fig. 6.

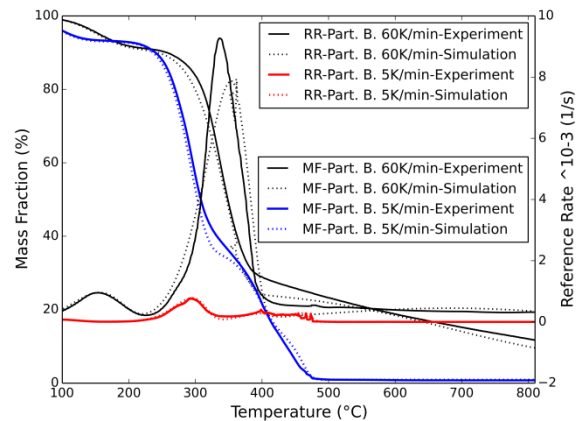


Figure 6: Comparison of particle board simulation and TGA

Furthermore, the user has to keep in mind that in this configuration of simulation only the pyrolysis behavior of the surface of materials is involved. For a more realistic pyrolysis simulation, the user should be informed about the pyrolysis depth, which

depends also on the thermal properties, specific heat, conductivity and density¹².

Thermal Properties

The influence of the thermal properties increases with the thickness of the material layer. Step by step the current simulation is adjusted to the real conditions of the experiments. To test the thermal properties, cone calorimeter experiments of the particle board and PMMA are modeled. Like the approach of modeling the TGA the focus of the cone simulation lies on the mass loss rate by the implementation of the delivered Arrhenius parameter before. The cone experiments are conducted with an external heat flux of 50 kW/m². Measurements of the temperature inside the sample in different distances to the surface record heating rates between 60 K/min to 80 K/min⁸. For this reason the TGA was also conducted with 60 K/min. Figures 7 and 8 show the results of the cone experiments compared to the simulation.

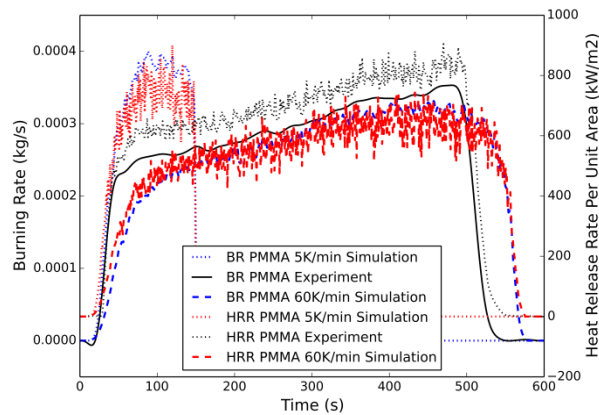


Figure 7: Comparison of PMMA simulation and Cone Calorimeter Experiment of 50kW/m²

It is obvious, that the simulation and experimental plots of the PMMA for a heating rate of 60 K/min is similar to the cone curve, while for the simulation based on 5 K/min only partly agreement at the time of ignition can be observed. The decomposition of PMMA can be limited to one reaction, shown by a heating rate of 60 K/min. In conclusion the reaction and corresponding Arrhenius parameter can be directly transferred from the TGA experiments to the cone calorimeter. Because of the negligible degradation steps of PMMA for lower heating rate the input parameters should be adapted to one reaction. Thus, the implementation of lower heating delivered Arrhenius parameter is also possible. Nevertheless, this approach works only for the characteristic fire behavior of PMMA. In contrast, the input parameters of the particle board are more influenced by the ambient conditions, like the heating rate. The charring process has to be considered for

the particle board as well as the thermal feedback, which is determined by the insulated backing of the sample. Although heating rates of 60 K/min to 80 K/min were measured in the sample during cone experiments, the TGA plot with a heating of 5K/min reflects the cone curve to a greater extent, figure 8. This can be explained by the volume of the sample: In the previous section it was discussed, that a high heating rate of the sample reduces the charring process, if a homogenous heating of the sample can be assumed. This applies to the little volume of the TGA (150 µl) but not for the cone sample (1.6E-04 m³). In contrast the slowly heating of the sample through the backside supports the charring process³. This effect should be included by an implementation of an additional charring process. As visualized in figure 8, the definition of the properties of the char and also the percentage of the mass influence the development of the mass loss rate considerably, even though the specific curves of the TGA experiments are identified by the FDS simulation. For this work only additional charring was considered, the Arrhenius parameter were not adjusted.

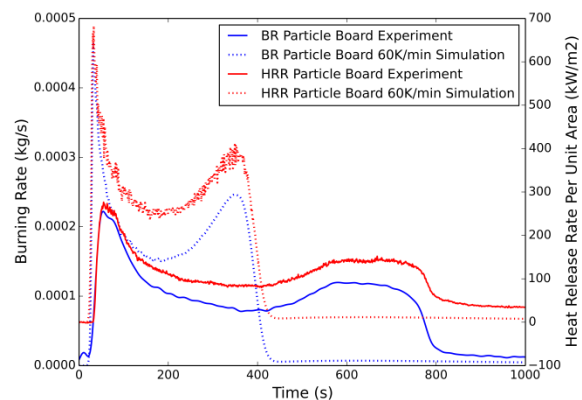
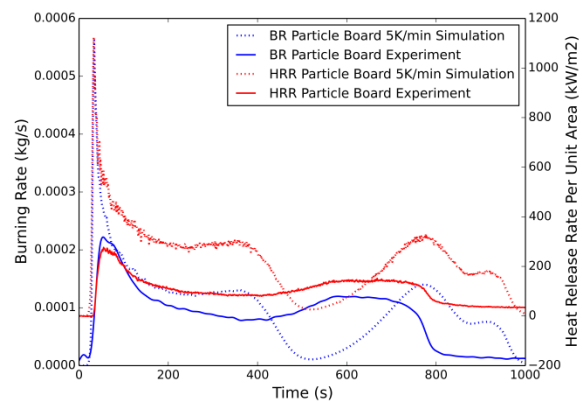


Figure 8: Comparison of particle board simulation and Cone Calorimeter Experiment of 50 kW/m²

In contrast to the TGA experiments, the thickness of the sample was modeled for the cone experiments,

this were 12mm for PMMA and 16mm for particle board. This additional model assumption enables to consider the variations of the specific heat, conductivity and density. Different tabled properties of PMMA^{3,2} are listed in table 3.

Table 3: Material properties of PMMA

Properties	Value
Density (g/cm ³)	1.18-1.19
Specific Heat Capacity (kJ/kg/K)	1.4-1.5
Thermal Conductivity (W/m/K)	0.167-0.25
Thickness (mm)	12
Heat of Combustion (MJ/kg)	24-26

Reducing the thermal responding behavior of the simulation by implementing the lower value of the conductivity (0.167 W/m/K) and a high specific heat (1.5 kJ/kg/K) leads to a decreasing heat release rate of 14% and a time delayed mass loss rate of 50s. On the other hand, an increased heat transfer coefficient of FDS leads to a more effective combustion. The same occurs by variations of the heat of combustion and heat of reaction. Those implemented simulation options of the more realistic configurations enable a detailed reproducing of the cone calorimeter experiments.

Scaling to real dimensions

From the steps described, received material properties are implemented in a fictive real scale scenario. A simple couch of PU and a chair of particle board are chosen to show the influences of the different input parameters.

Characterization of Combustion

In the previous section it was already specified, that not every reaction step can be reproduced. The following example shows the influence of ignoring the last and second reaction of the TGA curves of PU (fig. 1). The following series of pictures visualize the simulated fire spreading of a couch of PU with a different number of implemented reactions of the TGA curve.

By simulating a couch combustion with reduced number of reactions, the necessary endothermic energy (heat of reaction = 236 kJ/kmol¹³) of the pyrolysis process decreases. In conclusion, the fire spreads faster with a higher heat release rate. This effect needs to be considered by defining several numbers of reaction, degradation steps and especially the heat of reaction. In different literature^{4,13}, the heat of reaction of PU ranges between 300 and 2000 kJ/kmol. An implementation of a high value in the simulation leads to a limited combustion especially in combination with a low effective heat of combustion. With respect to literature references the

user can choose between wide ranges of properties linked to fire behavior.

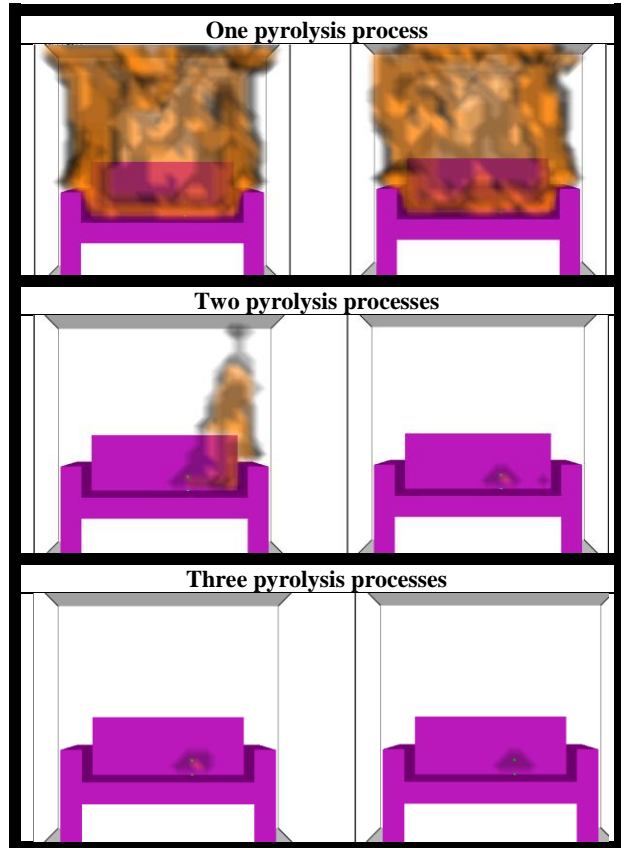


Figure 9: Simulated fire spreading after 20 s and 40 s depending on the reaction numbers

Likewise to the couch scenario, the fire spreading of the chair, which is build up with particle board, differs (see fig. 10). The focus lies on the comparison of the implemented Arrhenius parameters based on the TGA curves of particle board for the heating rate of 60 K/min and 5 K/min. Furthermore charring is also considered, based on the cone simulation.

Arrhenius parameters based on a heating rate of 5 K/min 60 K/min

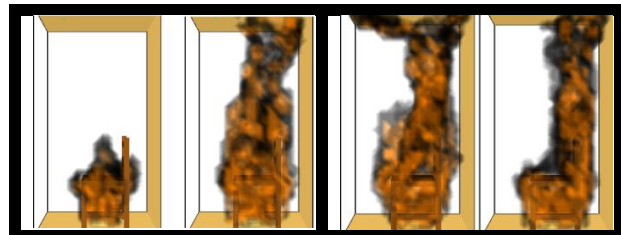


Figure 10: Simulated fire spreading after 240 s and 360 s depending on the Arrhenius parameter

The Arrhenius parameters, which are delivered from the higher heating rate of the TGA curves releases

about 700 kW, while the lower heating based Arrhenius parameters leads to a peak of 500 kW.

CONCLUSION

The user of fire simulations has to be aware of his responsibility to choose proper input parameters especially as he has to evaluate hazards of human beings. Furthermore, the investigation and definition of material properties from literature needs to be clarified (e.g. time of ignition of black PMMA by Cone Calorimeter Experiments according to ISO 5660...etc.) to minimize room for interpretation.

The transfer of material properties to different scales of fire scenario is limited. On the one hand, the pyrolysis and burning behavior of the materials varies depending on the boundary conditions. In this case the user should be aware to implement additional properties or processes, like charring. On the other hand the test methods differ from the simulating scenario, that does not agree with the ambient condition, like the thickness of the material or the ambient oxygen concentration. The consequences of different delivered material properties by testing with only one changing configuration (e.g. heating rate) lead to a complete change in fire behavior. The user needs to have a lot of experience to choose realistic simulation assumptions. The diversity of input parameters received by experiments, the way of implementing them into the simulation as well as other adjustments made by handling the different models lead to significant deviations in simulation results. A quantification of the different influences needs to be a future topic of research.

Today the user can simulate the same fire scenario by adjusting parameters as a worst case or as harmless based on legitimately references. The choice of input parameter has to be dependent on the specific fire scenario and the modeling procedure has to be transparent and clarified.

REFERENCES

- ¹ Camillo, A. (2013), "Multi-scale investigation of fire behaviour of a seat and a wall panel from European railway transport system", ENSMA
- ² Comuce M., Rogaume T.*, Richard F., Luche J. and Rousseaux P.(2010), "Kinetics and Mechanisms of the Thermal Degradation of Polymethyl Methacrylate by TGA/FTIR Analysis", Presentation of 6th International Seminar on Fire and Explosion Hazards, Leeds, UK

- ³ Hirschler, M. M., Morgan, A. B. (2008), "Thermal Decomposition of Polymers", SFPE Handbook of Fire Engineering, 4.Ed., 1/112-1/139
- ⁴ Jiang, Y. (2006), "Decomposition, Ignition and Flame Spread on Furnishing Materials", Centre for Environment Safety and Risk Engineering, Victoria University, Australia
- ⁵ Karastergiou, P.S., Philippou, J.L. (2000), "Thermogravimetric Analysis of Fire Retardant Treated Particleboards", Wood and Fire Safety, 385-394
- ⁶ McGrattan, K., Hostikka, S., McDermott, R., Floyd, J., Weinschenk, C., Overholt, K. (2014), "Fire Dynamics Simulator User's Guide", NIST Special Publication 1019 Sixth Edition
- ⁷ Meunders, A., Schroeder, B., Baker, G., Arnold, L., Pau, D., Spearpoint, M. (will published 2014), "Parameter Optimization and Sensitivity Analysis for Fire Spread Modelling with FDS ", SFPE 10th International Conference on Performance-Based Codes and Fire Safety Design Methods, University of Queensland, Australia
- ⁸ Pitts, W. M. (2011), "Applied Heat Flux Distribution and Time Response Effects on Cone Calorimeter Characterization of a Commercial Flexible Polyurethane Foam", Fire Technology, 50, 635-672, Springer
- ⁹ Pitts, W. M. (2013), "Role of two stage pyrolysis in fire growth on flexible polyurethane foam slabs", Fire and Materials, 38, 323-338
- ¹⁰ Plagge, M. (2011), "Simulation der Pyrolyse ausgewählter Feststoffe mit dem Programm gpyro und Vergleich mit Versuchsergebnissen, Thesis, Hochschule Magdeburg-Stendal, Germany
- ¹¹ Prasad, K., Kramer, R., March, N., Nyden, M., Ohlemiller, T., Zammarano, M., (2009) "Numerical Simulatoin of Fire Spread on Polyurethane Foam Slabs", 11th International Fire and Materials Conference, 697-708, San Francisco, USA

- ¹² Torero, J. L. (2008), "Flaming Ignition of Solid Fuels", SFPE Handbook of Fire Engineering, 4.Ed., 2/260-2/277
- ¹³ Valencia, L. B. (2009), Experimental and numerical investigation of the thermal decomposition of materials at three scales: application to polyether polyurethane foam used in upholstered furniture, Université de Poitiers